

Propylbenzene
103-65-1 | DTXSID3042219

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.68

Global applicability domain: Inside

Local applicability domain index: 6.41e-01

Confidence level: 6.41e-01

Nearest Neighbors from the Training Set

Image not found

Propylbenzene

Measured: 3.69

Predicted: 3.68

Image not found

Cumene

Measured: 3.66

Predicted: 3.77

Image not found

3-fluoropropylbenzene

Measured: 2.95

Predicted: 3.43

Image not found

4-Vinylcyclohexene

Measured: 3.93

Predicted: 3.82